Measurement-based Optimization via Tracking

B. Srinivasan and D. Bonvin

Institut d'Automatique

Ecole Polytechnique Fédérale de Lausanne

Lausanne, Switzerland

Objective

Optimal process operation in the presence of uncertainty

- In practice: Large amount of uncertainty possible
  - model mismatch
  - variable initial conditions
  - disturbances
- Key idea: Use measurements to combat uncertainty
- Question: How to ensure optimality from measurements without relying on a model?

Outline

- Review of optimization methodologies
- A tracking scheme to ensure optimality
- Examples
  - Chemical reactors
  - Inverted pendulum
- Conclusions

Optimization Methodologies
to Tackle Uncertainty

Problem: Optimization

Uncertainty: Nominal optimization (feasibility) | Optimization under uncertainty

$$\begin{aligned} \min_u \; & J = \phi(x,u) \\ s.t. \; & F(x,u,\theta^*) = 0 \\ & C(x,u) \le 0 \end{aligned}$$

Information: No measurement | Measurements

No measurement: Robust optimization (conservative)

$$\begin{aligned} \min_u \; & J = E[\phi(x,u)] \\ s.t. \; & F(x,u,\theta) = 0 \\ & \max_{\theta \in \Theta} C(x,u) \le 0 \end{aligned}$$

Measurements: Measurement-based optimization

Input calculation: Model-based | Model-free

Model-based (accuracy of model or persistency of excitation)

Model-free

Methodology:

Model-based:

$$\begin{aligned} \min_u \; & J = \phi(x,u) \\ s.t. \; & F(x,u,\hat{\theta}) = 0 \\ & C(x,u) \le 0 \end{aligned}$$

$$\begin{aligned} \hat{\theta} = \; & \arg\min_{\theta} \|y - \hat{y}\|_2 \\ s.t. \; & F(x,u,\hat{\theta}) = 0 \\ & \hat{y} = H(x,u) \end{aligned}$$

Model-free:

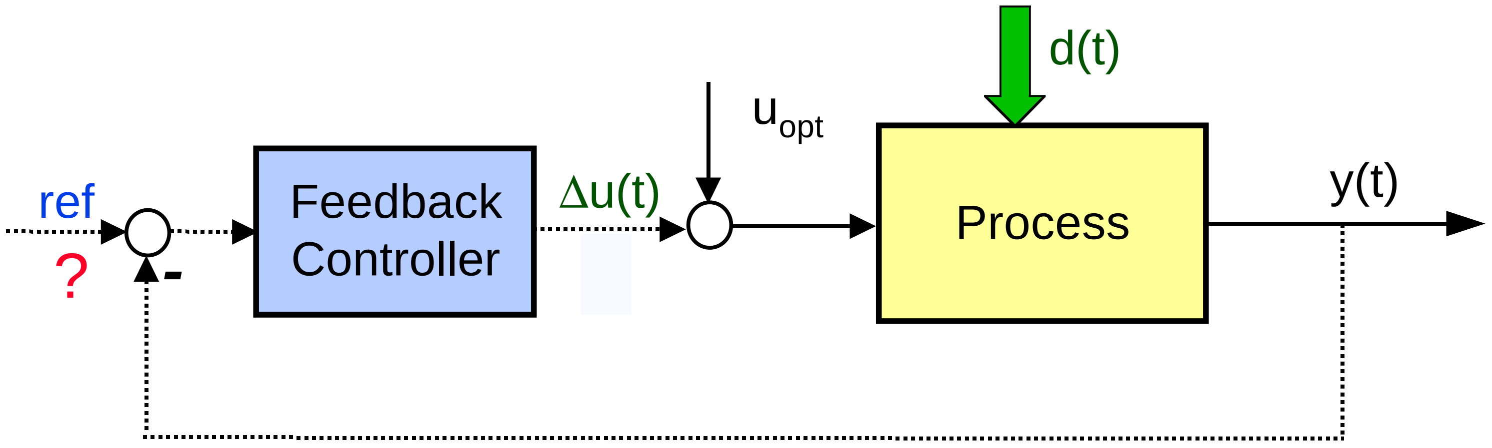
- Interpolation Evolution (curse of dimensionality)
- Reference tracking (what to track for optimality?)

Optimal Operation
under Uncertainty

Nominal model-based numerical optimization: u_{opt}

Uncertainty (model mismatch, disturbances): $\Delta u(t)$?

Optimal operation via tracking
- Use measurements and feedback to combat uncertainty
- Choice of reference ? - Invariant under uncertainty



Static Optimization Problem
Optimal Operating Point

$$\min_u J = \phi(x,u)$$
$$s.t. \qquad F(x,u) = 0$$
$$C(x,u) \le 0$$

- F - System at steady state
- C - Constraints
- Φ - Cost function
- u - Inputs -- decision variables

Decoupling Decision Variables

Reduced problem formulation

$$\min_{\pi} J = \phi(\pi)$$

$$\text{s.t.} \quad T(\pi) \le 0$$

Necessary conditions (NC)

$$\nu^T T = 0; \qquad \frac{\partial \phi}{\partial \pi} + \nu^T \frac{\partial T}{\partial \pi}\bigg|_{\pi^*} = 0$$

ν depends on uncertainty

ν can be eliminated from NC using knowledge of the active constraints T_a and decoupling of π

Compromise-seeking parameters

$$\tilde{\pi} \,/\!/\, T_a \qquad \frac{\partial T_a}{\partial \tilde{\pi}} = 0\,; \qquad \frac{\partial \phi}{\partial \tilde{\pi}}\bigg|_{\tilde{\pi}^*} = 0$$

Constraint-seeking parameters

$$\bar{\pi} \perp \tilde{\pi}; \quad \bar{\pi} = \frac{\partial T_a}{\partial \pi}\pi; \qquad T_a\big|_{\bar{\pi}^*} = 0$$

Optimization under Uncertainty

Conditions of optimality should be satisfied despite uncertainty

Decoupling of constraint-seeking
and compromise-seeking parameters

Constraints, sensitivities = 0

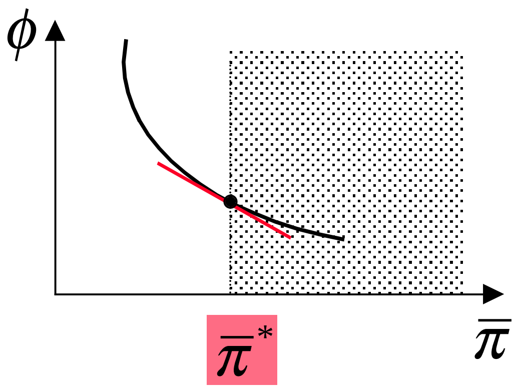
Availability of specific measurements

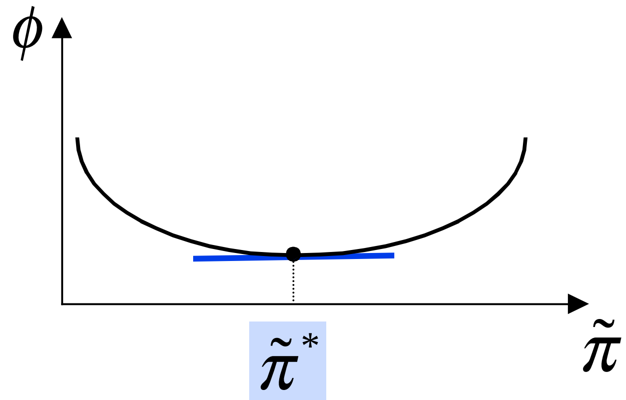
Track constraints and sensitivities

Assumption: The set of active constraints does not change

Variations in Cost

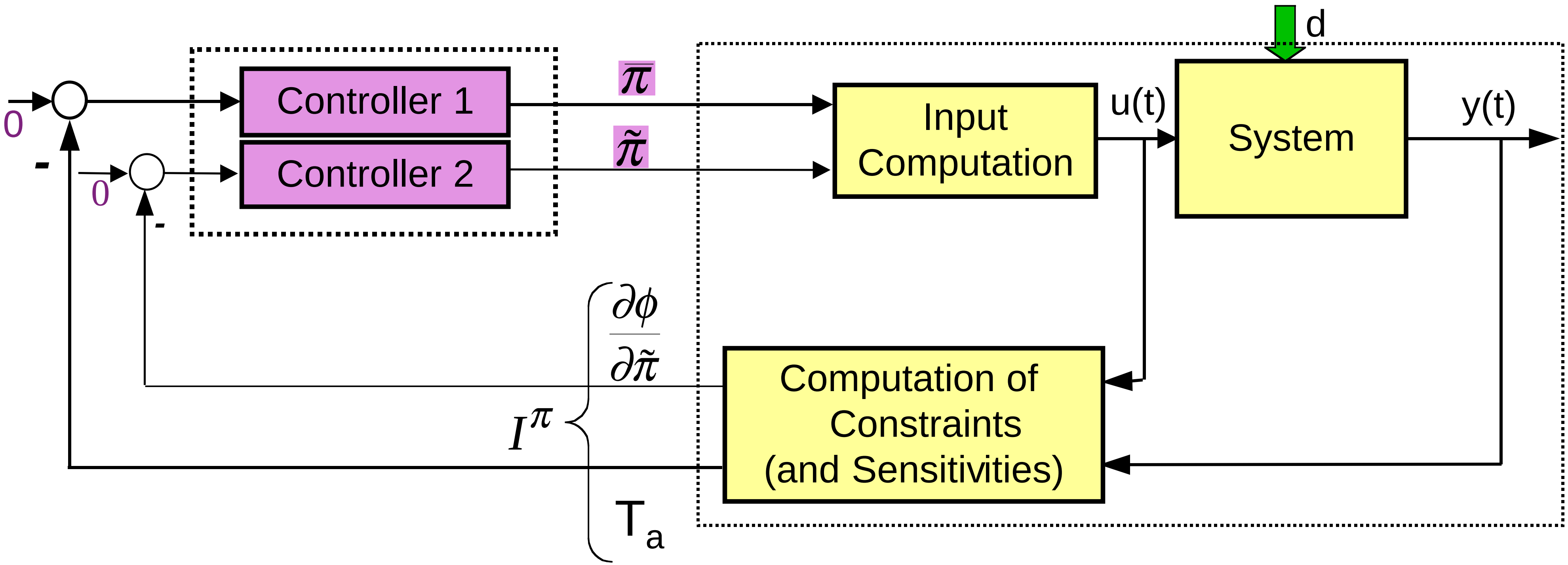
- Often high for deviations from constraints (T_a=0)
- Often low for deviations in sensitivities $\left(\frac{\partial \phi}{\partial \tilde{\pi}} = 0\right)$





Tracking constraints is often more important than regulating sensitivities

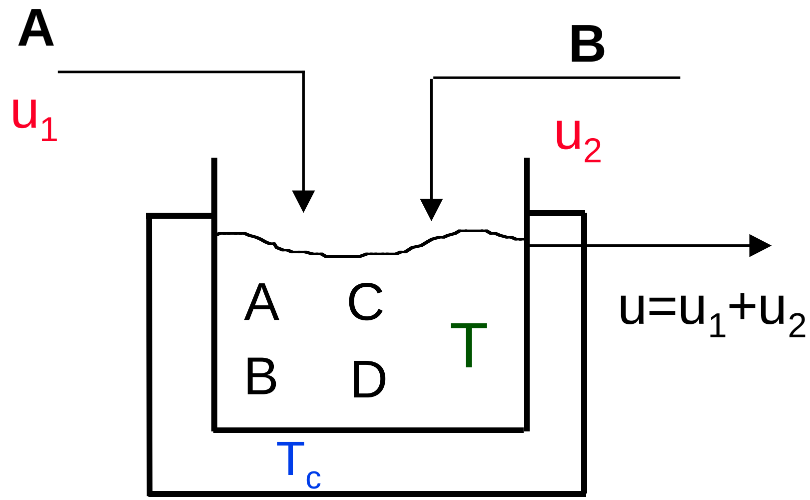
Tracking Invariants



Continuous Reactor

with Safety Constraints

$$A + B \xrightarrow{k_1} C$$
$$2B \xrightarrow{k_2} D$$



Exothermic reactions
Isothermal via adjustment of T_c

Objective: Maximize productivity of C by adjusting u_1 and u_2

Safety constraint: Heat removal limitation $q_{ex} \leq q_{ex,max}$

$$q_{rx} - q_{in} = q_{ex} = UA(T - T_c)$$

$q_{ex} \leq q_{ex,max}$ for $T_c \geq T_{c,min}$

Continuous Reactor

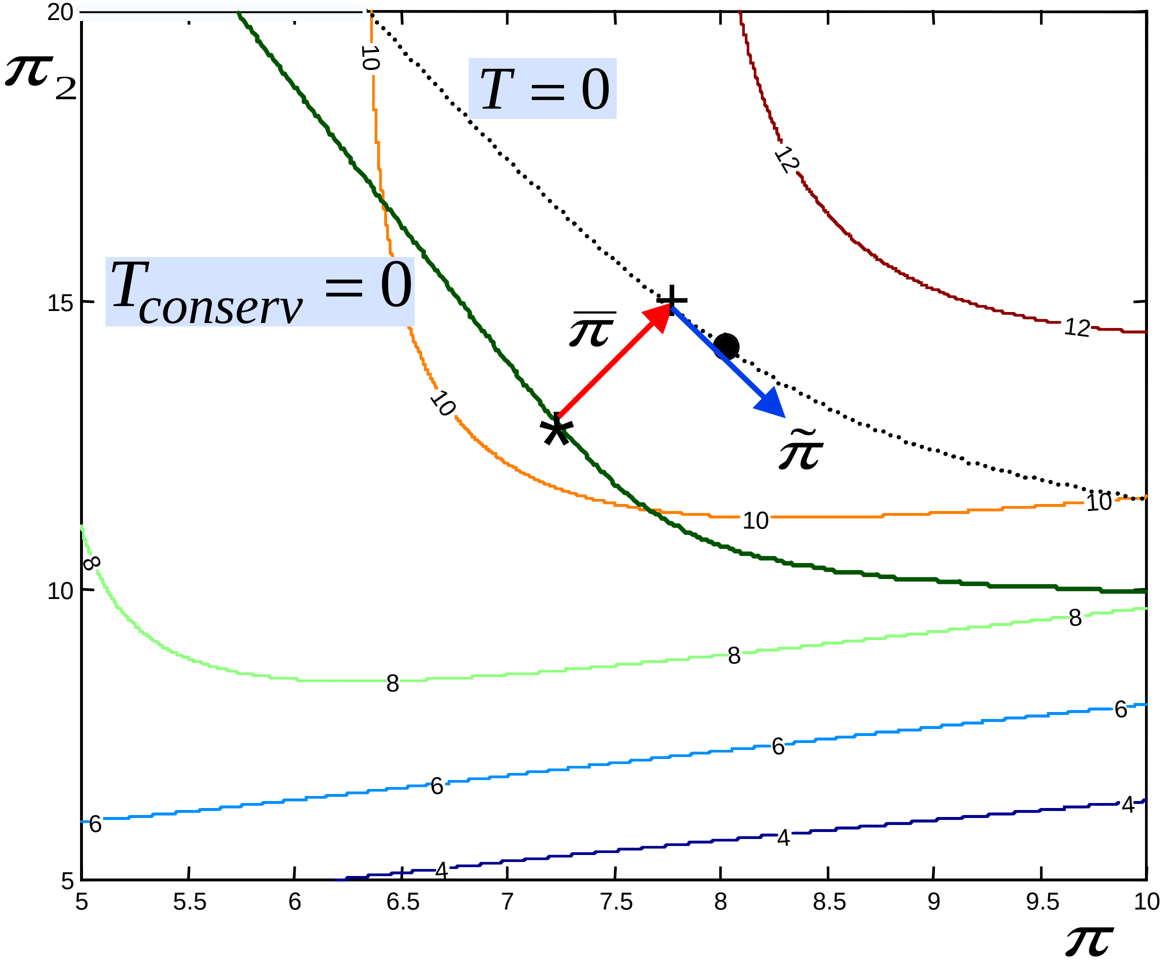
Various Scenarios

Reality: k_1=0.75 (unknown) Model: $0.4 \leq k_1 \leq 3$

1. No measurement
   Conservative solution

2. Measurement of constraint
   Adjustment of $\bar{\pi}$ to satisfy $T_c = T_{c,min}$

3. Measurement of constraint and sensitivity
   Adjustment of $\bar{\pi}$ and $\tilde{\pi}$



Continuous Reactor
Optimization Results

Optimization Scenario	**Constraint** $T_c \geq 10$ °C	**Cost** (mol of C)	**Loss** (%)
Open-loop Conservative optimal input	12.21	10.35	7.43
Measurement of constraint Adaptation of $\bar{\pi}$	10.00	11.17	0.01
Measurement of constraint and sensitivity Adaptation of $\bar{\pi}$ and $\tilde{\pi}$	10.00	11.18	0

Dynamic Optimization Problem

Optimal Operating Profiles

$$\min_{u(t)} J = \phi(x(t_f))$$

$$s.t. \qquad \frac{dx}{dt} = F(x,u) \qquad x(0) = x_0$$

$$S(x,u) \le 0$$

$$T(x(t_f)) \le 0$$

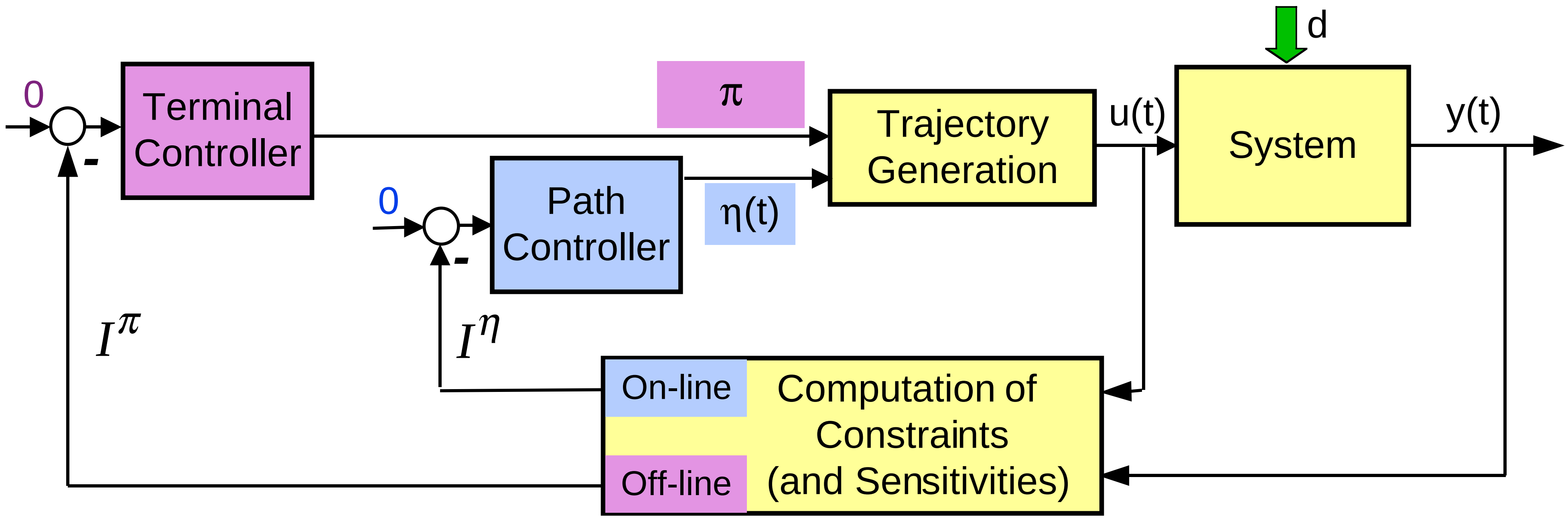
- F - Dynamic system
- S - Path constraints
- T - Terminal constraints
- Φ - Terminal cost
- u - Inputs -- decision variables
- t_f - Final time -- finite

Decoupling Decision Variables

Decision variables $u(t)$

- Decoupling in time → **Path objectives**: arcs $\eta(t)$
  - constraint-seeking var. $\bar{\eta}(t)$: $S_a=0$
  - compromise-seeking var. $\tilde{\eta}(t)$: $\lambda^T F_u=0$
- Static decoupling → **Terminal objectives**: parameters π
  - constraint-seeking var. $\bar{\pi}$: $T_a=0$
  - compromise-seeking var. $\tilde{\pi}$: $\dfrac{\partial\phi(x(t_f))}{\partial\tilde{\pi}}=0$

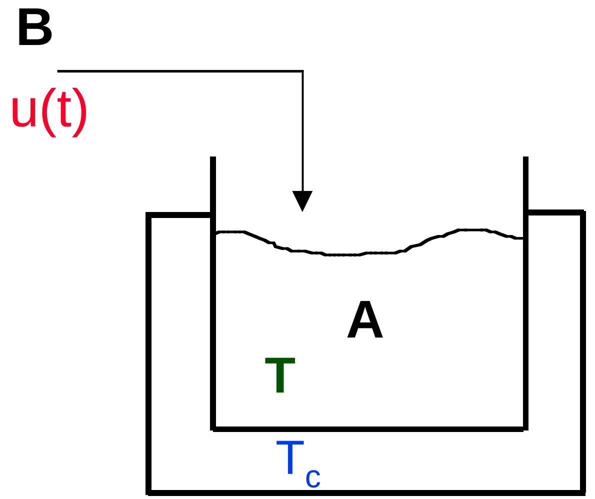
Tracking Invariants



Semi-batch Reactor

with Selectivity and Safety Constraints

$$A + B \xrightarrow{k_1} C$$
$$2B \xrightarrow{k_2} D$$



Exothermic reactions

Isothermal via adjustment of T_c

Objective: Maximize number of moles of C at t_f by adjusting u(t)

Safety path constraint: Heat removal limitation $T_c \geq T_{c,\min}$

Selectivity terminal constraint: Number of moles of D at t_f $n_{Df} \leq n_{Df,max}$

Semi-batch Reactor

Various Scenarios

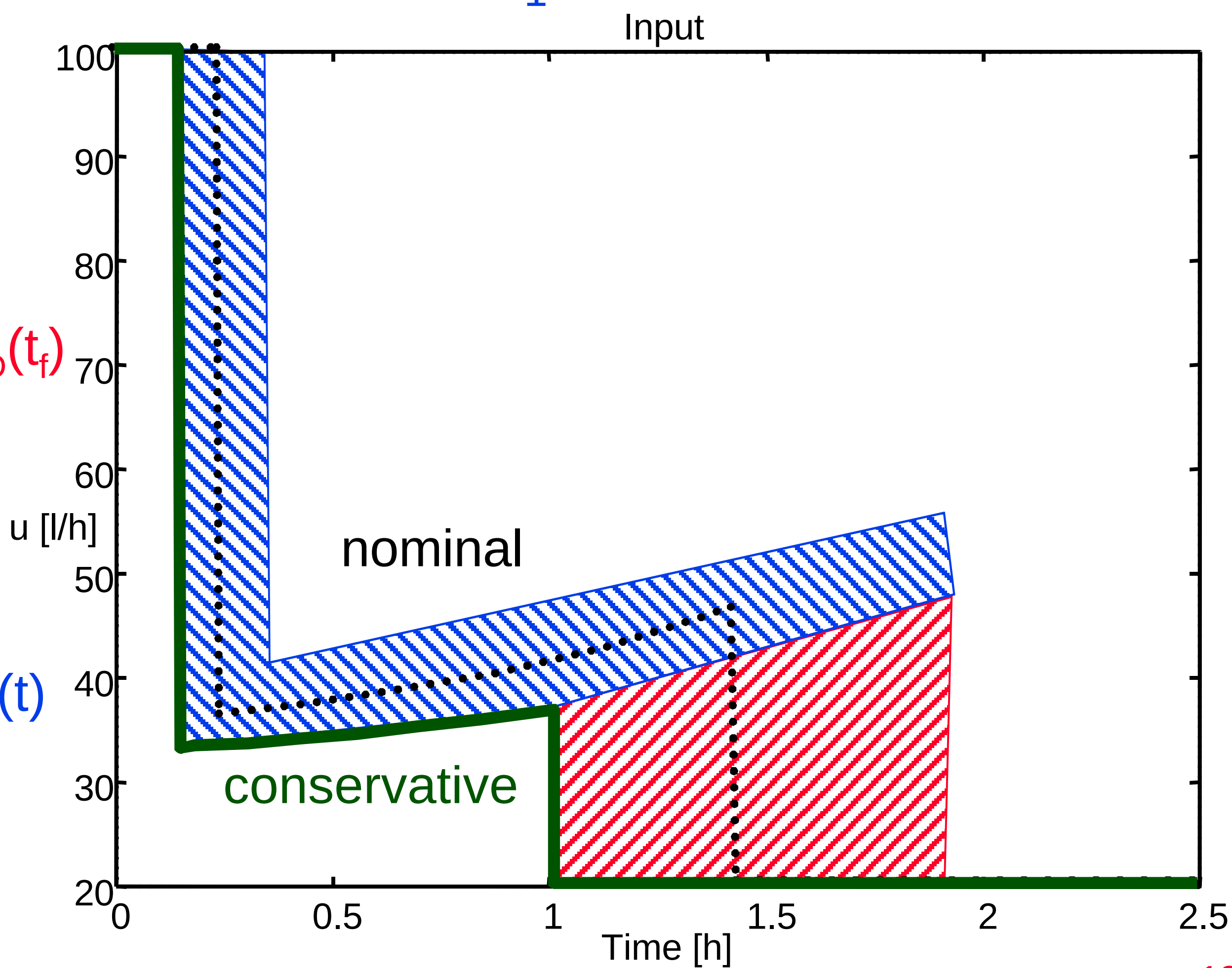
Reality: k_1=0.75 (unknown)

Model: $0.4 \leq k_1 \leq 1.2$

1. No measurement
   Conservative solution

2. Batch-end measurement of $n_D(t_f)$
   Adjustment of t_2 to
   satisfy $n_D(t_f)=n_{Df,max}$

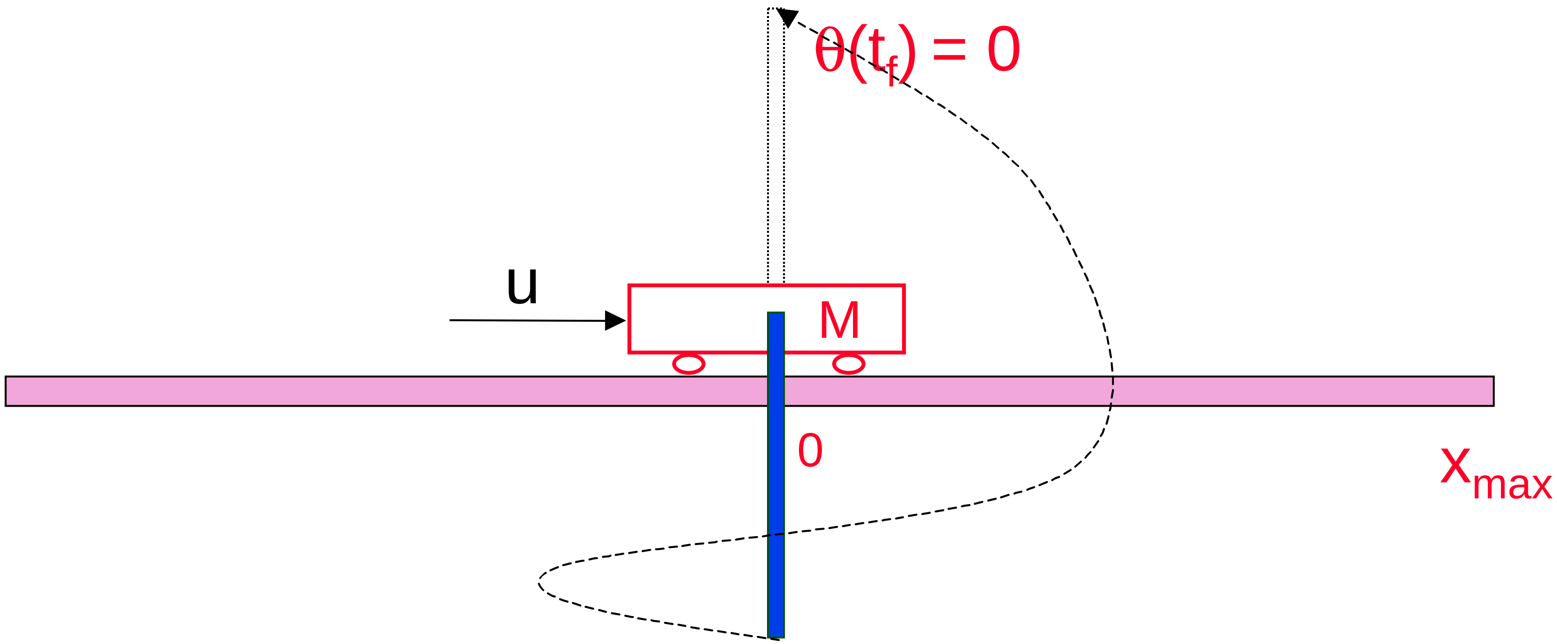
3. Measurement of $n_D(t_f)$ and $T_c(t)$
   Adjustment of t_2 and
   $u_{path}(t) = PI(T_{c,min}-T_c(t))$



Semi-batch Reactor
Optimization Results

Optimization Scenario	**Terminal Constraint** $n_D(t_f) \leq 5$ mol	**Path Constraint** $T_c(t) \geq 10$ °C	**Cost** (mol of C)	**Loss** (%)
Open-loop Conservative optimal input	2.71	12.87	498.8	20
Batch-end measurement Adaptation of t_2	5.00	11.50	589.2	2
On-line and batch-end measurements Adaptation of $u_{path}(t)$ and t_2	5.00	10.00	600.5	0.02

Inverted Pendulum on a Cart



Objective: Minimize the time to swing up: $\theta(t_f) = 0$

Path constraint: Length of the rail holding the cart: $|x(t)| \leq x_{max}$

Terminal constraint: Speed of the pendulum at t_f: $|\omega(t_f)| \leq \omega_{f,max}$

Inverted Pendulum

Various Scenarios

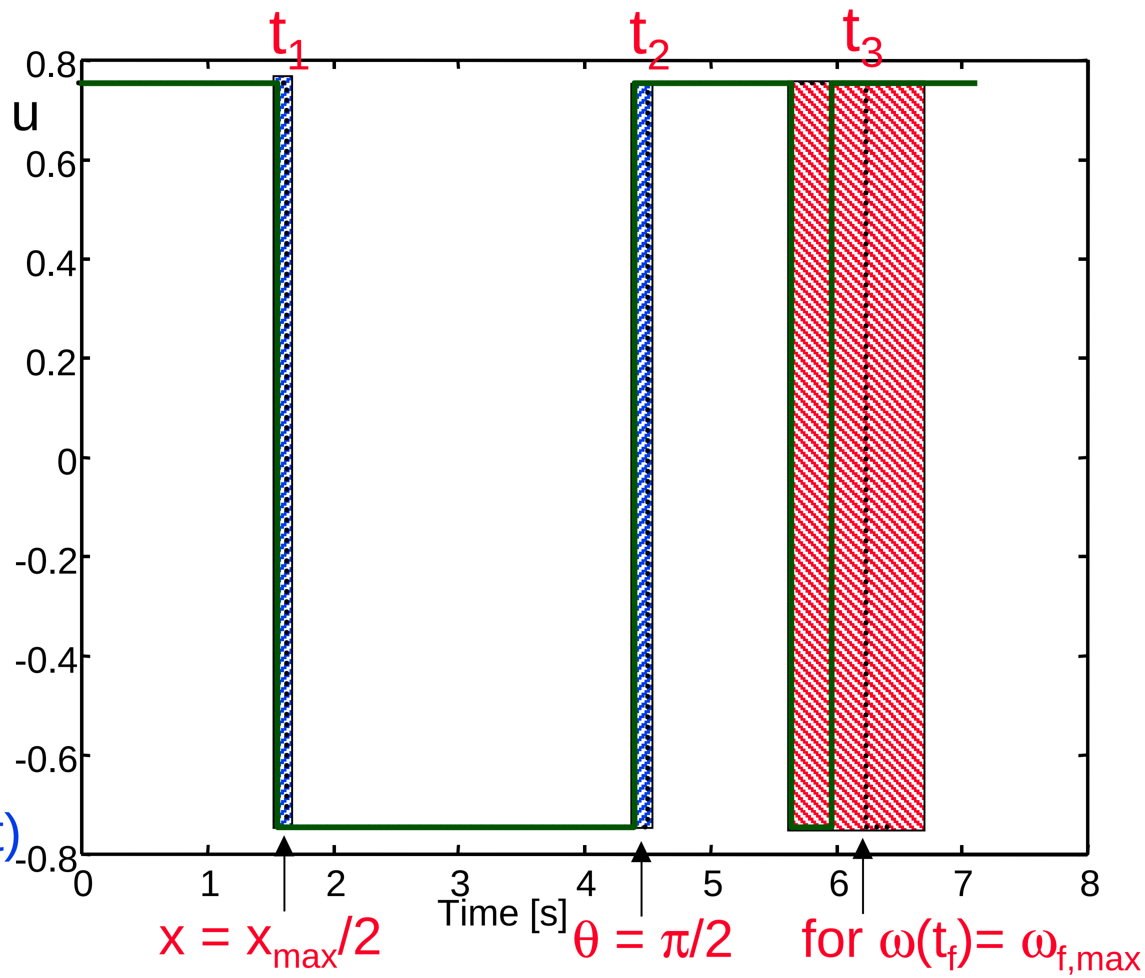
Reality: M=1.03 (unknown)

Model: $0.95 \le M \le 1.05$

1. No measurement
   Conservative solution

2. Measurement of $\omega(t_f)$
   Run-to-run adjustment of t_3 to satisfy $\omega(t_f) = \omega_{f,max}$

3. Measurement of $x(t)$, $\omega(t)$, $\theta(t)$
   Adjustment of t_1, t_2, and t_3
   Prediction: $\omega^2(t_f) = \omega^2(t) - 2\, a_{max}\theta(t)$



Inverted Pendulum
Optimization Results

Optimization Scenario	**Terminal Constraint** $\omega(t_f) \leq 0.71$ rad/s	**Path Constraint** $x(t) \leq 2$ m	**Cost** (s)	**Loss** (%)
Open-loop Conservative optimal input	0.69	1.8	7.18	11.4
Measurement of $\omega(t_f)$ Run-to-run adaptation of t_3	0.71	1.8	6.58	2.0
Measurements during the run Adaptation of t_1 , t_2, and t_3	0.71	2.0	6.45	0.1

Conclusions

- Presence of uncertainty
  - Calls for a paradigm shift in process optimization

    From "model-based" to "measurement-based"

  - Real process (and not model) used for optimization
- Model
  - Only used to determine the structure of the optimal inputs
  - Detailed model with accurate parameter values not necessary
- Measurement of constraints
  - Backoff to remain feasible in case of measurement errors
  - Reduced backoff compared to open-loop optimal inputs